APSC 143 – Introduction to Programming for Engineers

Assignment 9 - Recursion

Figure 1: What do chemists do? NewScientistsJobs (2019)

Objective:

Students will display their knowledge of recursion functions (and previous course topics) in programming using a real-world example, by developing a time step simulation program.

Problem:

You are part of a Queen's engineering design team that is working on a chemical cleaner to help industries reduce their environmental footprint. To find the most effective reactions for the cleaner, several chemical processes are being analyzed. Currently, the team is studying the oxidation of ammonia, which is described by the following reaction formula:

$$4\,NH_3 \;+\; 3\,O_2 \rightarrow 2\,N_2 \;+\; 6\,H_2O$$

One of the key characteristics of a chemical process is the rate at which the reaction occurs, known as the **reaction rate**, measured in (mol/L)/s, or M/s. This rate can be determined from the rate law of the reaction, which is shown below:

$$rate \;=\; k[NH_3][O_2]^2 \tag{1}$$

where **k = 9.65*10^{-2}**, [NH_3] is the current ammonia concentration, and [O_2] is the current oxygen concentration. Equation 1 allows us to calculate the reaction rate at any step of the reaction, including the initial rate. The rate can then be used to determine the change in concentration for each reactant and each product over a given time step (usually a fraction of a second):

$$rate = -\frac{\Delta[NH_3]}{4\Delta t} = -\frac{\Delta[O_2]}{3\Delta t} = \frac{\Delta[N_2]}{2\Delta t} = \frac{\Delta[H_2O]}{6\Delta t} \qquad (2)$$

Note that **the rate of reaction is not** constant, because the concentration of the reactants is decreasing over time, and the reaction rate is directly related to those concentrations. So, the reaction rate will **also** decrease over time. Each time the change in reactant concentrations is calculated using Equation 2, the rate will also need to be recalculated using those new reactant concentrations in Equation 1.

The team wants to ensure that the reaction is running at a rate of greater than 0.001 M/s. You want to know how long the reaction goes at a rate higher than 0.001 M/s, as well as the concentrations of all reactants and products once it reaches that point. It's your job to develop a program to determine these values before the experiment is conducted.

Instructions:

Below is a guideline for how to approach this problem, though you may choose to approach it however you wish. **Make sure to express your results using the format specified below**:

- Retrieve user input for the initial concentrations [NH_3] and [O_2]
- Call your recursive function `reaction()` to return the time it takes to reach a rate of 0.001 M/s **using a time interval of 0.01 s**
- Print the time to the console using the format specified below
- Write a **recursive** function named `reaction()` that does the following:
    - Compute the current reaction rate using Equation 1.
    - Check to see if the rate has decreased below 0.001 M/s.
        - If so, print the concentrations of the reactants & products and **return the time elapsed**.
    - Compute the change in concentration for each molecule based on the current rate using Equation 2.
    - Call the function with the new concentrations and increment the time by the time interval.

Comments are mandatory for this assignment. Add comments as necessary for key pieces in your code, such as variable declaration, conditional statements, and looping conditions to explain what the program is doing.

Your output must match the sample output below exactly; otherwise, the auto grading software will not be able to grade your assignment, which may affect your mark.

Sample Output:

(Note: You **DO NOT** need to print the values in bold; they are shown only to display the **scanf** input for this example.)

(Note: Make sure that every calculated value is printed to 2 decimal places, and that the last line also prints a new line.)

The below output displays the correct results for initial concentrations of 0.67 M for ammonia and 0.42 M for oxygen:

```
Enter initial ammonia and oxygen concentrations: 0.67 0.42

Final Reaction Molarities:

NH3: 0.34 M

O2:  0.17 M

N2:  0.16 M

H2O: 0.49 M

The reaction will take 26.23 seconds to reach a rate 0.001 M/s.
```

Submission Instructions:

Create your program using CLion and upload it here for grading. **Your program file must be named** "**apsc143assign9.c**" for your assignment to be graded. Do not include any personal information (student number, name, etc.) in your submission. Also, add a comment attesting to the originality of your work.

Refer to the assignment rubric on OnQ for a detailed breakdown of the grading criteria. Your submission must adhere to the assignment rules as outlined in the submission policy document for this course, which can also be found on OnQ. There is zero tolerance for plagiarism in this course. This auto grading software will automatically flag potential cases of plagiarism, which will be reviewed by the instructors.

More information on assignment submissions can be Found in Week 2, and information on the specific definition and repercussions of plagiarism can be found in the "Begin Here (About This Course)" module.